

=> fil reg

FILE 'REGISTRY' ENTERED AT 11:25:32 ON 21 DEC 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4

DICTIONARY FILE UPDATES: 19 DEC 2003 HIGHEST RN 628722-21-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

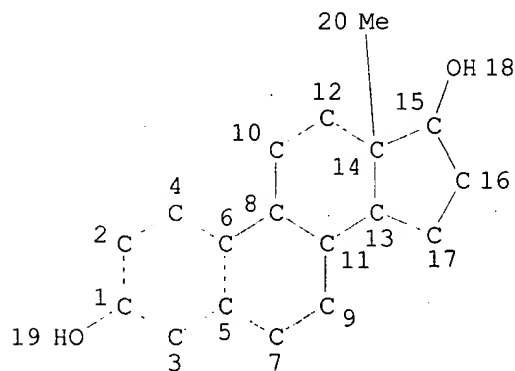
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 113

L1 STR



NODE ATTRIBUTES:

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 16

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

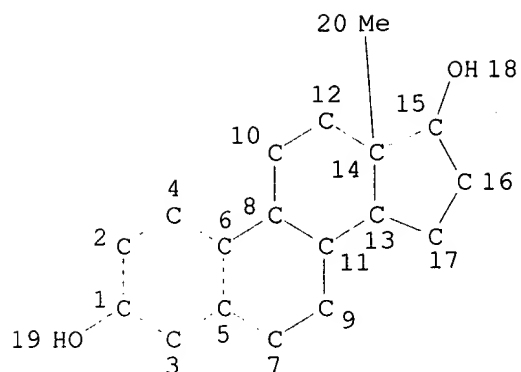
RSPEC 1

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L3 949 SEA FILE=REGISTRY CSS FUL L1

L4 STR



## NODE ATTRIBUTES:

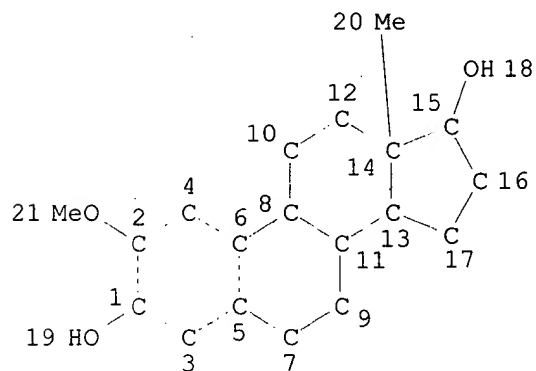
CONNECT IS M1 RC AT 2  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 1  
 NUMBER OF NODES IS 20

## STEREO ATTRIBUTES: NONE

L5 448 SEA FILE=REGISTRY SUB=L3 CSS FUL L4  
 L6 501 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT L5  
 L7 STR



## NODE ATTRIBUTES:

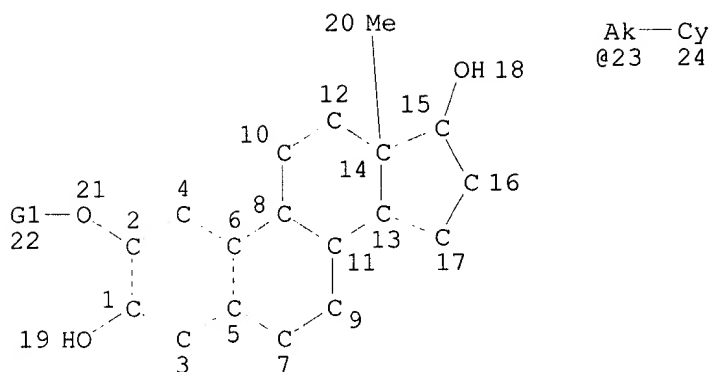
CONNECT IS M1 RC AT 16  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 1  
 NUMBER OF NODES IS 21

## STEREO ATTRIBUTES: NONE

L8 25 SEA FILE=REGISTRY SUB=L6 CSS FUL L7  
 L9 476 SEA FILE=REGISTRY ABB=ON PLU=ON L6 NOT L8  
 L10 STR



VAR G1=AK/23/CY

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 16

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L13 5 SEA FILE=REGISTRY SUB=L9 SSS FUL L10

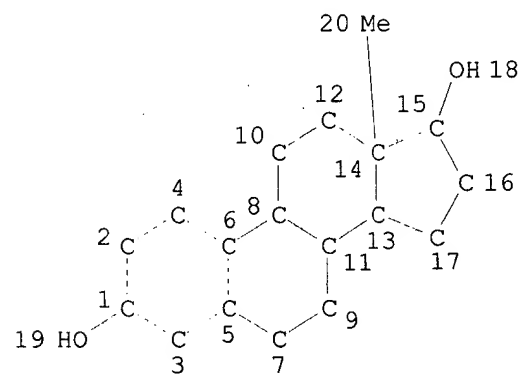
100.0% PROCESSED 23 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

=> d sta que 116

L1 STR



NODE ATTRIBUTES:

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 16

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

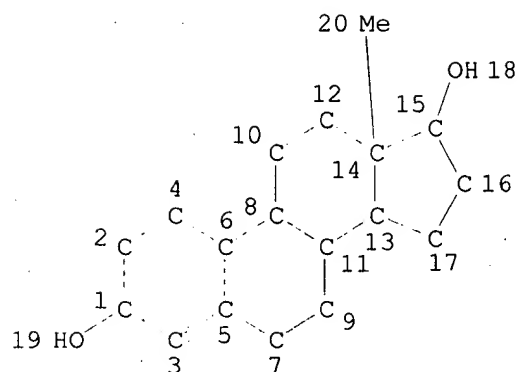
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L3 949 SEA FILE=REGISTRY CSS FUL L1

L4

STR



## NODE ATTRIBUTES:

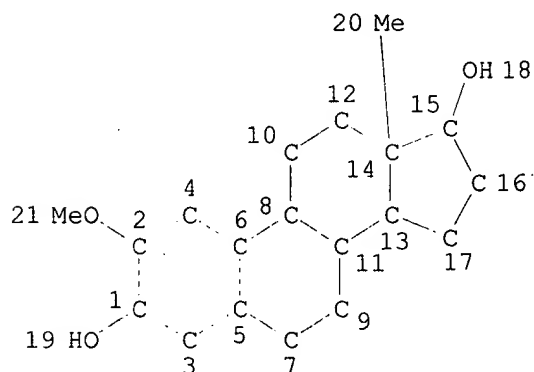
CONNECT IS M1 RC AT 2  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 1  
 NUMBER OF NODES IS 20

## STEREO ATTRIBUTES: NONE

L5 448 SEA FILE=REGISTRY SUB=L3 CSS FUL L4  
 L6 501 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT L5  
 L7 STR



## NODE ATTRIBUTES:

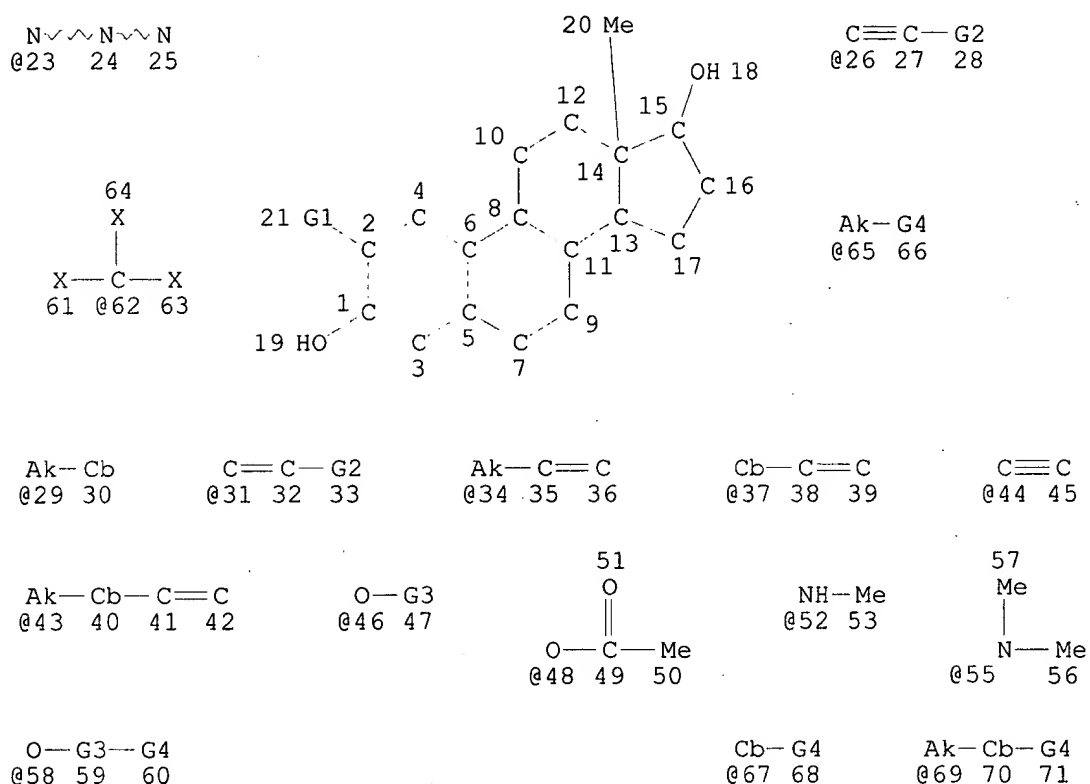
CONNECT IS M1 RC AT 16  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 1  
 NUMBER OF NODES IS 21

## STEREO ATTRIBUTES: NONE

L8 25 SEA FILE=REGISTRY SUB=L6 CSS FUL L7  
 L9 476 SEA FILE=REGISTRY ABB=ON PLU=ON L6 NOT L8  
 L14 STR



VAR G1=23/CN/26/31/34/37/43/44/46/48/CHO/NH2/52/55/58/65/67/69

VAR G2=AK/CB/29

VAR G3=AK/CB/29

VAR G4=OH/NH2/X/62

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 16

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 2

NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE

L16 3 SEA FILE=REGISTRY SUB=L9 SSS FUL L14

100.0% PROCESSED 476 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

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L13 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2003 ACS on STN

RN 202398-05-8 REGISTRY

CN  $\beta$ -D-Glucopyranosiduronic acid, (16 $\beta$ ,17 $\beta$ )-16-fluoro-3,17-dihydroxyestra-1,3,5(10)-trien-2-yl (9CI) (CA INDEX NAME)

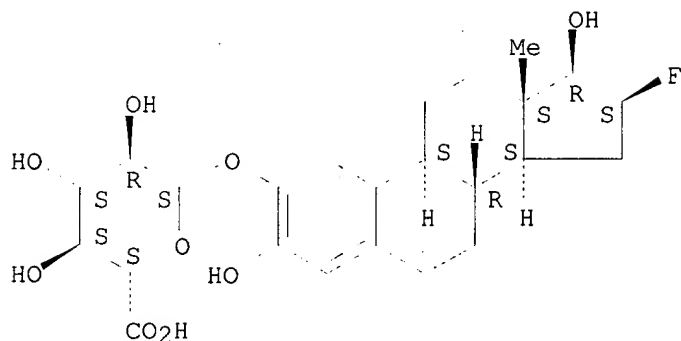
FS STEREOSEARCH

MF C24 H31 F O9

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



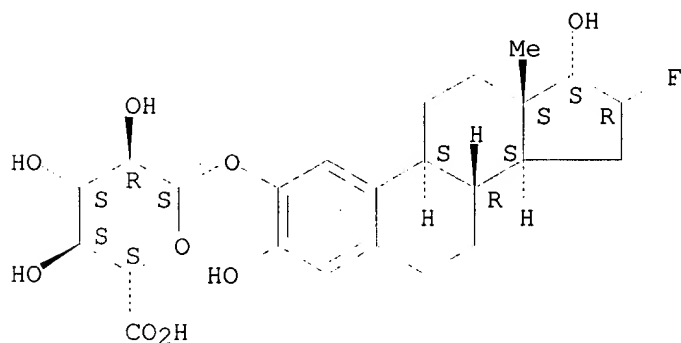
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:138115

L13 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 202397-99-7 REGISTRY  
CN  $\beta$ -D-Glucopyranosiduronic acid, (16 $\alpha$ ,17 $\alpha$ )-16-fluoro-3,17-dihydroxyestra-1,3,5(10)-trien-2-yl (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H31 F O9  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

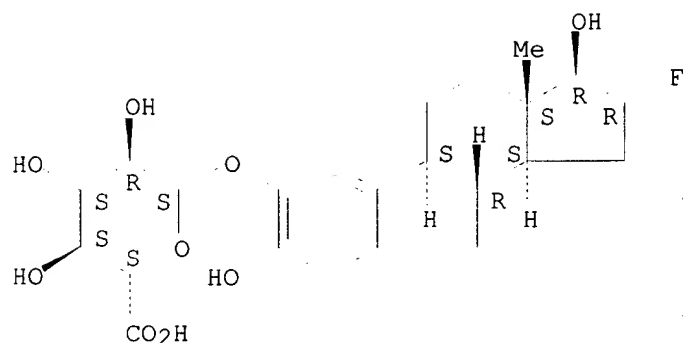
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:138115

L13 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 202397-95-3 REGISTRY  
CN  $\beta$ -D-Glucopyranosiduronic acid, (16 $\alpha$ ,17 $\beta$ )-16-fluoro-3,17-dihydroxyestra-1,3,5(10)-trien-2-yl (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H31 F O9

SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

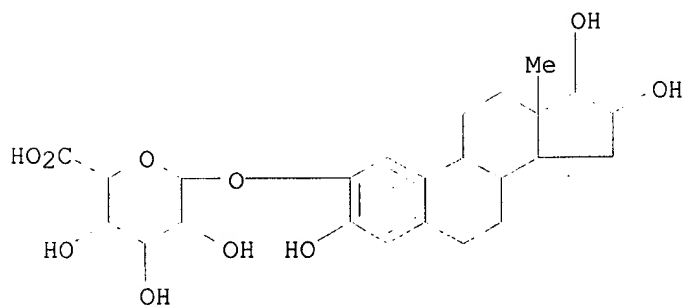
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:138115

L13 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 116408-03-8 REGISTRY  
CN  $\beta$ -D-Glucopyranosiduronic acid, (16 $\alpha$ ,17 $\beta$ )-3,16,17-trihydroxyestra-1,3,5(10)-trien-2-yl, monosodium salt (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

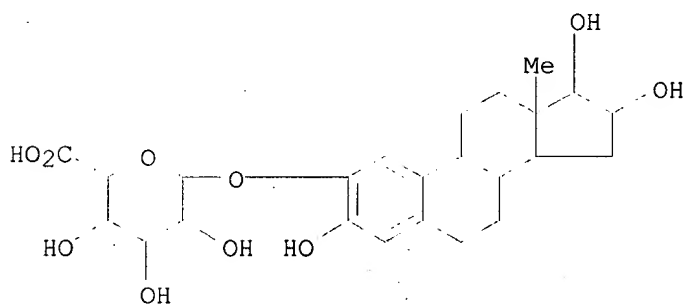
CN Estrane,  $\beta$ -D-glucopyranosiduronic acid deriv.  
MF C<sub>24</sub> H<sub>32</sub> O<sub>10</sub> . Na  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)  
CRN (55349-22-9)



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 109:129502

L13 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 55349-22-9 REGISTRY  
CN  $\beta$ -D-Glucopyranosiduronic acid, (16 $\alpha$ ,17 $\beta$ )-3,16,17-  
trihydroxyestra-1,3,5(10)-trien-2-yl (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Estrane,  $\beta$ -D-glucopyranosiduronic acid deriv.  
OTHER NAMES:  
CN 2-Hydroxyestriol 2-glucuronide  
MF C24 H32 O10  
CI COM  
LC STN Files: BEILSTEIN\*, BIOBUSINESS, CA, CAPLUS, CASREACT, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)  
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

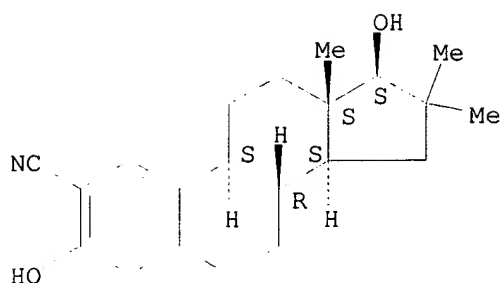
REFERENCE 1: 114:43278  
REFERENCE 2: 114:722  
REFERENCE 3: 112:112186  
REFERENCE 4: 110:154664  
REFERENCE 5: 87:63000  
REFERENCE 6: 83:53697

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L16 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 258278-72-7 REGISTRY  
CN Estra-1,3,5(10)-triene-2-carbonitrile, 3,17-dihydroxy-16,16-dimethyl-,  
(17 $\beta$ )- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN EM 1926  
FS STEREOSEARCH  
MF C21 H27 N O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.





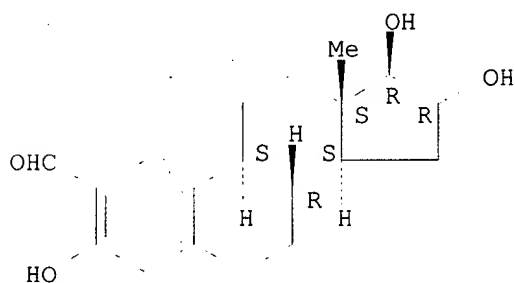
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:152024

L16 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2003 ACS on STN.  
RN 123715-87-7 REGISTRY  
CN Estra-1,3,5(10)-triene-2-carboxaldehyde, 3,16,17-trihydroxy-,  
(16 $\alpha$ ,17 $\beta$ )- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C19 H24 O4  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 111:233337

L16 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 88599-96-6 REGISTRY  
CN Estra-1,3,5(10)-triene-3,16,17-triol, 2-amino-, (16 $\alpha$ ,17 $\beta$ )-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C18 H25 N O3  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Absolute stereochemistry.